Comment on "Variation of the superconducting transition temperature of hole-doped copper oxides".

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We point out the incorrect derivation of the gap equation in X.-J. Chen and H. Q. Lin [Phys. Rev. B **69**, 104518 (2994)] within the interlayer tunneling (ILT) model for multilayered cuprates. There, the *local* structure in **k**-space of the ILT effective interaction has not been taken into due account when the ILT model is generalized to the case of n layers per unit cell. This is a specific characteristic of the ILT model that, apart from giving rise to a highly nontrivial **k**-dependence of the gap function, is known to enhance the critical temperature T_c in a natural way. As a consequence, we argue that Chen and Lin's results cannot be employed, in their present form, for a quantitative interpretation of the high-pressure dependence of T_c in Bi-2212, as is done by X.-J. Chen *et al.* [`cond-mat/0408587`, to appear in Phys. Rev. B]. Moreover, when the generalization of X.-J. Chen *et al.* [`cond-mat/0408587`] is applied to the case $n = 2$, it fails to reproduce the original ILT gap equation. However, a more careful analysis of the ILT model for multilayered cuprates, taking into account the nonuniform hole distribution among inequivalent layers, has been earlier suggested to describe the observed pressure dependence of T_c in homologous series of high-T_c cuprates.

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In Ref. 1, Chen and Lin reconsider the dependence of T_c on doping and on the number of layers in a homologous series of multilayered high-T_c cuprates within the interlayer tunneling (ILT) model [2]. However, in deriving their gap equation, Chen and Lin erroneously neglect the intrinsic *local* structure in momentum (**k**) space of the effective ILT coupling. This is a specific characteristic of the ILT model, which is known to give rise to highly nontrivial features in the **k**-dependence of the gap function already for a bilayer complex [3, 4]. Moreover, a local term in the gap equation has been shown to provide a lower bound for T_c at all dopings, which is the precise way in which the ILT mechanism enhances T_c [3]. The consequences of such an incorrect analysis of the ILT model are both qualitative and quantitative. Therefore, the recent use of Chen and Lin's results to interpret the high-pressure dependence of T_c in Bi-2212 [5] can be questioned. In this context, we point out that a more careful analysis of the ILT model for layered cuprates has been presented elsewhere [6], and successfully applied to study the pressure dependence of T_c in homologous series of layered cuprates, by explicitly taking into account the inhomogeneous hole-doping in inequivalent layers [7, 8].

Superconductivity in the high-T_c layered cuprates is characterized by *(i)* a non-monotonic dependence of T_c on the overall hole-doping δ; *(ii)* a monotonic increase of T_c with the number of layers n, for moderately low n ($n \lesssim 3$). While *(i)* is a generic consequence of the quasi-bidimensional nature of these compounds (see *e.g.* Ref. 9), the latter fact has suggested that coherent tunneling of superconducting pairs between adjacent CuO_2 layers may considerably enhance T_c [2]. Within the ILT model, it is postulated that strong in-plane correlations forbid coherent hopping of single particles between adjacent CuO_2 planes. Such a restriction is removed when accessing the superconducting state, where interlayer Josephson tunneling of Cooper pairs is allowed. This results in a net gain in kinetic energy, as compared to the normal state. Thus, within the ILT model, superconductivity is stabilized *via* a kinetic mechanism, as opposed to conventional BCS superconductivity, where the enhancement in kinetic energy is overcompensated by a reduction in the potential energy [10].

However, after its original formulation more than a decade ago [2], the relevance of the ILT mechanism at least for single-layer cuprates has been called into question by experiments [11, 12]. Recently, Chakravarty *et al.* [13] have revived the ILT model in connection with multilayered cuprates. There, ILT needs not be the sole source of superconducting condensation energy. Charge carriers require a 'seed' in-plane interaction to form Cooper pairs in a given symmetry channel, before they can actually tunnel between adjacent layers [3]. Such in-plane interaction would then provide the missing condensation energy [13].

Moreover, it has been suggested that the competition

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with a 'hidden' order parameter, such as a d-density-wave (dDW) [14], could be responsible for the downturn of T_c with n, for $n \gtrsim 3$. Indeed, in multilayered cuprates, due to the different proximity to the 'charge reservoir' blocks, experiments [15] as well as density functional theory calculations [16] revealed a nonuniform hole-content distribution between inner and outer layers. Since this usually places inner (outer) layers in the underdoped (overdoped) region of the cuprate phase diagram, competition with the dDW order would be stronger in inner layers than in outer layers, thus depressing T_c with increasing n. Hydrostatic pressure could then be used to tune both the overall hole-content content and its distribution among inequivalent layers, thus inducing an 'exchange of roles' between inner and outer layers with respect to the onset of superconductivity [7], which is observed as 'kinks' in the pressure dependence of T_c in layered cuprates [8].

The effective Hamiltonian considered by Chen and Lin [1] (see also [3, 7]) is

$$\begin{aligned} H &= \sum_{\ell \mathbf{k}\sigma} \xi_{\mathbf{k}} c^{\ell\dagger}_{\mathbf{k}\sigma} c^{\ell}_{\mathbf{k}\sigma} - \sum_{\ell \mathbf{k}\mathbf{k}'} V_{\mathbf{k}\mathbf{k}'} c^{\ell\dagger}_{\mathbf{k}\uparrow} c^{\ell\dagger}_{-\mathbf{k}\downarrow} c^{\ell}_{-\mathbf{k}'\downarrow} c^{\ell}_{\mathbf{k}'\uparrow} \\ &\quad + \sum_{\langle \ell\ell' \rangle} \sum_{\mathbf{k}} T_J(\mathbf{k}) c^{\ell\dagger}_{\mathbf{k}\uparrow} c^{\ell\dagger}_{-\mathbf{k}\downarrow} c^{\ell'}_{-\mathbf{k}\downarrow} c^{\ell'}_{\mathbf{k}\uparrow}, \end{aligned} \tag{1}$$

where $\xi_{\mathbf{k}}$ is the in-plane quasiparticle dispersion measured with respect to the chemical potential μ^{ℓ} ($\mu^{\ell} \equiv \mu$ for all layers, in Ref. 1), and $c^{\ell\dagger}_{\mathbf{k}\sigma}$ is a quasiparticle creation operator with wave-vector $\mathbf{k}$ and spin σ on layer ℓ. It should be emphasized that in Eq. (1) the first interaction term ($V_{\mathbf{k}\mathbf{k}'}$) pertains to a single layer and governs the overall symmetry of the order parameter (*i.e.*, d-wave, if $V_{\mathbf{k}\mathbf{k}'} = V g_{\mathbf{k}} g_{\mathbf{k}'}$, with $g_{\mathbf{k}} = \frac{1}{2}(\cos k_x - \cos k_y)$) [17], while the second term applies to adjacent layers $\langle \ell\ell' \rangle$, and is *local* in $\mathbf{k}$-space, with $T_J(\mathbf{k}) = \frac{1}{16} T_J (\cos k_x - \cos k_y)^4$ [2]. This enforces momentum conservation for the interlayer pair tunneling process. (The effect of $\mathbf{k}$-space broadening of the ILT kernel, *e.g.* due to impurities, has been considered in Ref. 18.)

A straightforward mean-field analysis of Eq. (1) for a bilayer complex and an in-plane superconducting instability in the d-wave channel yields the gap equation [3]:

$$\Delta_{\mathbf{k}} = \frac{\Delta_0 g_{\mathbf{k}}}{1 - T_J(\mathbf{k}) \chi_{\mathbf{k}}}, \tag{2}$$

where Δ_0 is determined self-consistently from

$$1 = \frac{V}{N} \sum_{\mathbf{k}'} g^2_{\mathbf{k}'} \frac{\chi_{\mathbf{k}'}}{1 - T_J(\mathbf{k}') \chi_{\mathbf{k}'}}. \tag{3}$$

Here, $\chi_{\mathbf{k}} = (2E_{\mathbf{k}})^{-1} \tanh(\beta E_{\mathbf{k}}/2)$ is the pair susceptibility at the inverse temperature $\beta = (k_{\rm B}T)^{-1}$, $E_{\mathbf{k}} = \sqrt{\xi^2_{\mathbf{k}} + |\Delta_{\mathbf{k}}|^2}$ is the upper branch of the superconducting spectrum, and N is the number of lattice sites.

Eqs. (2) and (3) should be immediately compared and contrasted with Eq. (9) in Ref. 1 (for a multilayered complex) and Eq. (1) in Ref. 5 (for a bilayer complex). Even without going into the subtleties of the more general derivation for an n-layered complex (for which, see Refs. 6, 7), or with the competition among several in-plane pairing channels (Ref. 3), it is apparent that the gap function within the ILT model, Eq. (2), is characterized by a *local* prefactor $[1 - T_J(\mathbf{k})\chi_{\mathbf{k}}]^{-1}$ which, albeit linked self-consistently to Δ_0 *via* Eq. (3), is responsible of most of the quantitative and qualitative features of the model. Such a structure is missing in Refs. 1, 5. Even though the actual symmetry of the gap function is independent of the ILT kernel, and is rather determined by the d-wave nature of the in-plane coupling, the ILT mechanism endows the gap function with a nontrivial structure in $\mathbf{k}$-space [3], which has been shown to be consistent with ARPES results [4]. Moreover, the 'renormalized' pair susceptibility in the summand of Eq. (3), *viz.* $\chi_{\mathbf{k}} \mapsto \chi_{\mathbf{k}}/[1 - T_J(\mathbf{k})\chi_{\mathbf{k}}]$, which is due to the local ILT tunneling amplitude, gives rise to additional, algebraic divergences in the energy dependence of the integrated pair susceptibility, as opposed to the logarithmic one, typical of BCS theory [19]. This is directly responsible of the enhancement of T_c within the ILT model. In particular, in the case of a bilayer complex, one analytically finds a lower bound for T_c as

$$k_{\rm B}T^*(\mu) = \begin{cases} \dfrac{T_J}{64} \left(\dfrac{\mu_\perp - \mu}{\mu_\perp + 2t} \right)^4, & \mu_\perp \le \mu < \mu_{\rm VH}, \\ \dfrac{T_J}{64} \left(\dfrac{\mu_\top - \mu}{\mu_\top - 2t} \right)^4, & \mu_{\rm VH} \le \mu \le \mu_\top, \end{cases} \tag{4}$$

where nearest (t) and next-nearest (t') hopping have been assumed, and $\mu_\perp = -4t + 4t'$, $\mu_\top = 4t + 4t'$, and $\mu_{\rm VH} = -4t'$ denote the bottom, the top of the band, and the location of the Van Hove singularity, respectively [3].

On the contrary, the ILT kernel enters Chen *et al.*'s gap equation in Eq. (9) of Ref. 1 and Eq. (1) of Ref. 1 as an additional contribution to the non-local in-plane coupling term, *i.e.* it amounts to defining another in-plane interaction, with no reference to interlayer tunneling. *This same observation applies to the general case of an n-layered complex.* In that case, the gap equation for each layer should also contain a local contribution due to the ILT mechanism between adjacent layers (again, absent in Ref. 1), with an ILT renormalized pair susceptibility $\chi^{\ell}_{\mathbf{k}}/[1 - T_J(\mathbf{k})\hat{\chi}^{\ell}_{\mathbf{k}}]$ for each layer [6, 7], with

$$\begin{aligned} \hat{\chi}^{\ell}_{\mathbf{k}} &= \left[\sin\left(\frac{\ell\pi}{n+1} \right) \right]^{-1} \left[\chi^{\ell+1}_{\mathbf{k}} \sin\left(\frac{(\ell+1)\pi}{n+1} \right) \right. \\ &\quad \left. + \chi^{\ell-1}_{\mathbf{k}} \sin\left(\frac{(\ell-1)\pi}{n+1} \right) \right], \end{aligned} \tag{5}$$

which can be further simplified in the limit of uniform hole-content in all layers (as is tacitly assumed in Ref. 1). In analogy to the bilayer case, the condition

$$\min_{\mathbf{k}} [1 - T_J(\mathbf{k}) \chi^{\ell}_{\mathbf{k}}] = 0 \tag{6}$$

then implicitly defines a lower bound $T^{*\ell}_c$ for the critical temperature corresponding to the onset of superconductivity *in the given layer* ℓ. Therefore, for nonuniform

hole-content among inequivalent layers, as is the case for the multilayered cuprates [15, 16], one can estimate a lower bound to T_c as $\max_\ell T_c^{*\ell}$. A nonuniform distribution of the overall hole-content among inequivalent layers can be conveniently described by means of appropriate models [7]. This then enables us to identify whether the superconducting instability first sets in in inner or outer layers. One finds a crossover as function of the overall hole-content [7], which has been related to the observed 'kinks' in the pressure dependence of T_c in several layered cuprates [8].

In conclusion, we have pointed out an incorrect derivation of the gap equation(s) for layered cuprates within the ILT model [1, 5] for the general case of n superconducting layers per unit cell. This in turn leads to a failure to capture most of the qualitative and quantitative features of the theory, both for bilayered and multilayered compounds. As a consequence, the theoretical analysis of the high pressure data in Ref. 5 is not consistent with the ILT mechanism. On the other hand, a more careful analysis of the ILT model [6], when taking into account a nonuniform hole-content distribution among inequivalent layers [7], is indeed able to reproduce the observed pressure dependence of T_c in multilayered cuprates [8].

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